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ITERATIVE METHODS FOR LARGE LINEAR AND NONLINEAR LEAST  
SQUARES PROBLEMS(U) RICE UNIV HOUSTON TEX DEPT OF  
MATHEMATICAL SCIENCES J E DENNIS 31 MAR 86

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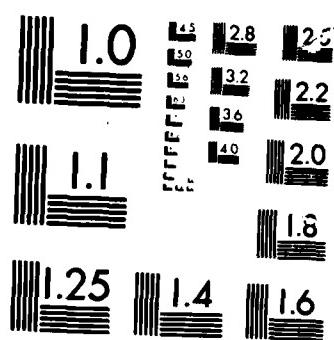
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20. ABSTRACT (Continue on reverse side if necessary and identify by block number) <b>This grant provided support to 8 graduate students. Of these, 4 have received their Ph.D.'s and the other 4 will have graduated by Fall of 1987. With so many graduate students involved, the research pursued has necessarily been very broad within optimization. The most exciting accomplishment is a new trust region approach to global convergence for nonlinear programming problems. Testing has also begun on a variable metric variant of the Karmarkar linear programming algorithm that could be of great practical significance if very preliminary tests are any indication. Other interesting work has been a unified convergence</b>		

ITERATIVE METHODS FOR LARGE LINEAR AND NONLINEAR  
LEAST SQUARES PROBLEMS

Final Report

John E. Dennis

March 31, 1986

U. S. Army Research Office

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## TECHNICAL SUMMARY

This grant provided support to 8 graduate students. Of these, 4 have received their Ph.D.'s and the other 4 will have graduated by Fall of 1987. With so many graduate students involved, the research pursued has necessarily been very broad within optimization. - The most exciting accomplishment is a new trust region approach to global convergence for nonlinear programming problems. Testing has also begun on a variable metric variant of the Karmarkar linear programming algorithm that could be of great practical significance if very preliminary tests are any indication. Other interesting work has been a unified convergence analysis for the many variants of the conjugate gradient method, a convergence analysis of the popular Nelder-Mead algorithm, a novel use of interactive computer graphics to obtain user preferences in multi-objective optimization, a convergence analysis of the EM algorithm for mixture density estimation, and a survey of all the work done by researchers in various fields on nonlinear programming problems in which some subset of the variables always appear linearly.

The original proposal was mostly concerned with ideas developed in a joint paper with Dr. Trond Steihaug who left Rice to return to Norway and work for Statoil. The paper will appear in Siam Journal for Numerical Analysis. It suggests several ways to attack the large sparse nonlinear least squares problem by column grouping schemes connected to graph coloring which are generally used to cheaply compute large sparse Jacobian approximations. Our results were interesting but we chose not to follow them further because of more promising avenues of research. One sidelight suggested by a referee for the paper is that our ideas could be used to find orderings for SOR for large linear least squares problems. Again the results were interesting but not compelling.

The most exciting research is reported on in the joint paper with Maria Rosa Celis and Richard Tapia. We found a conceptually simple and elegant way to get around the main problem people have encountered in trying to extend trust region methods to constrained optimization. That problem is that the approximating QP might not be feasible (this is a problem with the SQP approach) or that even if the QP is feasible, there may not be a feasible point inside the trust region. Our way around both these difficulties is to make use of some convergence results for the trust region algorithms applied to finding a nonlinear feasible point. Standard theorems show that if we ask for some percentage of at least as much linear feasibility in the Euclidean norm as would be given by the steepest descent step for the Gauss-Newton quadratic model for the sum-of-squares of constraints, then we will converge to a feasible point of the nonlinear constraints with a standard trust region implementation. We minimize a quadratic model of the Lagrangian subject to this local constraint. An interesting benefit of this approach is that the multiplier of the 'sufficiently feasible' local constraint is a penalty constant for the augmented Lagrangian which can then be naturally available as a merit function.

In our test results, we found that this 'full' trust region step performs very well in the majority of cases, but sometimes we have trouble computing the step with our modified More-Hebden-Reinsch iteration. This has motivated us to seek for a dogleg implementation of the above idea. We are

testing such an algorithm now.

The first student supported by this contract was Professor Richard Hathaway, currently in the Statistics Department at the University of South Carolina. His thesis built on work begun in my previous ARO contract to prove that a certain reasonable regularization of the mixture density problem made it well posed without inhibiting the EM algorithm generally used for practical applications.

Dr. Teresa Parks wrote an interesting thesis on optimization problems in which some of the variables can be eliminated by writing a closed form solution for them at the optimum in terms of the other variables. The simplest example is the so-called VARPRO or separable least squares problem in which one has a nonlinear least squares problem with some linear variables. In such a case, one can formally eliminate the linear variables by writing them in terms of a projection that depends on the nonlinear variables. This gives a new lower dimensional optimization problem to solve. If there are constraints involved, this approach can backfire. Simple bound constraints on the linear variables are quite common in such problems and they can be transformed into very nonlinear constraints on the remaining variables when the linear variables are eliminated. Dr. Parks found many connections among published works in this area which seem not to have been noticed before.

The central difficulty with the Karmarkar algorithm for practical linear programming is the solution of a large sparse linear least squares problem. We are currently testing a BFGS type method for updating an approximation to this projection matrix in order to cut the cost of this part of the algorithm. So far, we have only test results for a single small problem, but they are excellent. We are currently debugging a sparse version of the algorithm.

We have gotten some very interesting results on conjugate directions methods and on the Nelder-Mead simplex algorithm. The work on conjugate directions is based on a new and simple way of viewing the large number of algorithms that go by the name. We prove convergence of all the methods at once in a shorter clearer proof than is generally given for any one of them. This work is joint with Kathryn Turner, a graduate student supported by this grant, who should finish her degree this May.

The work on the Nelder-Mead algorithm is joint with Dr. Dan Woods, who received his degree with support from this grant in May '85. We are still improving our results, but they constitute the first convergence results, both positive and negative, ever obtained for this much used algorithm.

The heavy usage of this algorithm in practice would be reason enough to analyze it, but my interest is heavily influenced by my interest in exploring the use of such pattern search algorithms in parallel optimization. Virginia Torczon will explore this area for her Ph.D. thesis.

Karen Williamson made progress in developing a parameter estimation routine for inverse problems for ODE's. She has now begun to consult with one of our chemical kinetics researchers on some meaningful test problems.

The final graduate student being supported by this grant is Michael Lewis. Mr. Lewis has a very strong background in traditional PDE's which he gained at the University of Minnesota. We have been considering the infinite dimensional Broyden method approach suggested by Griewank and Kelley and Sachs. This is a very promising approach to solving nonlinear differential equations numerically.

PUBLICATIONS BY J.E.Dennis, Jr.

- (1) (with R.B. Schnabel) *Numerical Methods for Unconstrained Optimization and Nonlinear Equations*, Prentice-Hall (1983), 378 pp.
- (2) (with H.F. Walker) Inaccuracy in Quasi-Newton Methods: Local Improvement Theorems, *Math. Prog. Study 22*, pp. 70-85.
- (3) A User's Guide to Nonlinear Optimization Algorithms, *Proceedings of the IEEE 72*, pp. 1765-1776.
- (4) (with M.R. Celis and R.A. Tapia) A Trust Region Strategy for Equality Constrained Optimization, in *Numerical Optimization 1984*, ed. by P.T. Boggs, R.H. Byrd and R.B. Schnabel, SIAM, pp. 71-82.
- (5) (with H.F. Walker) Least-Change Secant Update Methods with Inaccurate Secant Conditions, *SIAM J. on Numerical Analysis 22*, pp. 760-778.
- (6) (with T. Steihaug) On the Successive Projections Approach to Least-Squares Problems, Rice MASC TR 83-18 (to appear in *SIAM J. on Numerical Analysis*).
- (7) (with Sheng Songbai and Phuong Vu) A Memoryless Augmented Gauss-Newton Method for Nonlinear Least Squares, Rice MASC TR 85-1, submitted for publication.
- (8) (with David M. Gay and Phuong Vu) A New Test System of Nonlinear Equations, Rice MASC TR 83-16, submitted for publication.
- (9) (with Kathryn Turner) Generalized Conjugate Directions, submitted for publication.
- (10) (with Daniel J. Woods) Convergence Properties of the Nelder-Mead Simplex Algorithm, in preparation.

## **PARTICIPATING SCIENTIFIC PERSONNEL**

- (1) Professor R.A.Tapia
- (2) Dr. Trond Steihaug, Statoil, Norway.
- (3) Richard Hathaway, Ph.D. 1984, currently at University of South Carolina (directed jointly with J.R. Thompson)
- (4) Maria Rosa Celis, Ph.D. 1985, currently AFSOR Postdoctoral at Rice (directed jointly with R.A. Tapia)
- (5) Teresa Parks, Ph.D. 1985, currently employed by Schlumberger (directed jointly with R.A. Tapia)
- (6) Daniel J. Woods, Ph.D. 1985, currently AFSOR Postdoctoral at Rice
- (7) Kathryn Turner, graduate student, Ph.D. expected 1986.
- (8) Karen Williamson, graduate student, Ph.D. expected 1987.
- (9) Virginia Torczon, graduate student, Ph.D. expected 1987.
- (10) Michael Lewis, graduate student, Ph.D. expected 1987.



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